

GMU-WM 2011 Workshop on Undergraduate Research in Computational Mathematics

Organized by

Department of Mathematics, College of William and Mary
Department of Mathematical Sciences, George Mason University

Sponsored by

National Science Foundation CSUMS program

Time: April 16, 2011

Location: Blow Hall Room 331, College of William and Mary

Program

Time	Chair	Speaker	Title
9:15-10:00			Registration, Breakfast
10:00-10:05	Junping Shi		Opening remarks
10:05-11:00	Paul Tian	Philip Maini	<i>Mathematical Models for Tumour Dynamics</i>
11:00-11:15			Coffee break
11:15-11:35	Tim Sauer	Kevin Talbott	<i>Modeling the Evaporation of a Tear Film Over a Contact Lens</i>
11:35-11:55		Olivia Walch	<i>Modeling Facilitation and Depression in Thalamocortical Relay Neurons</i>
11:55-12:15		Jeff Soosiah	<i>Perfect Partitioning of Sets of Permutations</i>
12:15-13:30			Lunch
13:30-13:50	Sarah Day	Ian Johnson	<i>Numerical continuation with the Diblock Copolymer Equation in one dimension</i>
13:50-14:10		Ben Holman	<i>Patterns in Extinction in Coupled Ricker Model</i>
14:10-14:30		Russell Mahoney	<i>Modeling of Interface-Dominated Materials Properties</i>
14:30-14:50		Ruoyan Sun	<i>Global Stability of Endemic Equilibrium of Multigroup SIR Model with Nonlinear Incidence</i>
14:50-15:05			Coffee break
15:05-15:25	Evelyn Sander	Ari Cukierman	<i>Vertex Identifying Codes</i>
15:25-15:45		Arjun Sanghvi	<i>A Stability Study of an Equilibrium Asset Price Model</i>
15:45-16:05		William Brayer	<i>An Agent-Based Modelling Approach to Financial Markets</i>
16:05-16:25		Georgia Pfeiffer	<i>Basins of attraction in stage structured populations</i>
16:25-16:40			Coffee Break
16:40-17:00	Junping Shi	Dian Yang	<i>A Solvable Hyperbolic Free Boundary Problem Modeling Tumor Regrowth</i>
17:00-17:20		Robert Hill	<i>Modeling Complex Physical Phenomena using Energy Minimization Principle</i>
17:20-17:40		Byong Kwon	<i>Computational Docking of Molecular Wires to the Reaction Center of Rhodobacter Sphaeroides</i>
17:40-18:00		Matt Peppe	<i>Assortativity in Networks of Neurons</i>
18:30			Dinner at Food for Thought

Participant List

Student

- William Brayer (George Mason University)
- Ari Cukierman (College of William and Mary)
- Robert Hill (George Mason University)
- Ben Holman (College of William and Mary)
- Ian Johnson (George Mason University)
- Byong Kwon (George Mason University)
- Russell Mahoney (George Mason University)
- Matt Peppe (College of William and Mary)
- Ankit Patel (College of William and Mary)
- Georgia Pfeiffer (College of William and Mary)
- Austin Powell (College of William and Mary)
- Arjun Sangvhi (George Mason University)
- Jeff Soosiah (College of William and Mary)
- Patrick Steel (College of William and Mary)
- Ruoyan Sun (College of William and Mary)
- Kevin Talbott (George Mason University)
- Rachel Taylor (College of William and Mary)
- Dian Yang (College of William and Mary)
- Olivia Walch (College of William and Mary)
- Cayla Wallwork (College of William and Mary)

Faculty:

- Dan Anderson (Math, George Mason University)
- Sarah Day (Math, College of William and Mary)
- Anne Fernando (Math, Norfolk State University)
- Robert Michael Lewis (Math, College of William and Mary)
- Rex Kincaid (Math, College of William and Mary)
- Drew LaMar (Applied Science, College of William and Mary)

- Larry Leemis (Math, College of William and Mary)
- Rom Lipcius (Marine Science, College of William and Mary)
- David Phillips (CS/Math, College of William and Mary)
- Philip Maini (Math, Oxford University)
- Evelyn Sander (Math, George Mason University)
- Tim Sauer (Math, George Mason University)
- Leah Shaw (Applied Science, College of William and Mary)
- Junping Shi (Math, College of William and Mary)
- Greg Smith (Applied Science, College of William and Mary)
- Jianjun Paul Tian (Math, College of William and Mary)
- Daniel Vasiliu (Math, Christopher Newport University)
- Tom Wanner (Math, George Mason University)
- Zhifu Xie (Math, Virginia State University)

Abstract of the Talks (in the order of presentation)

Philip Maini Oxford University, UK (Keynote Speaker)

Mathematical Models for Tumour Dynamics

The complex interaction of the multitude of physical and biochemical processes that lead to tumour invasion are too difficult to understand by verbal reasoning alone. As a result, the field of mathematical oncology is growing very fast. In this talk, mathematical models for tumour invasion, somatic evolution and tumour vasculature dynamics will be presented. They will consist of systems of partial differential equations, cellular automata and hybrid models. The results will be compared to experiment and therapeutic consequences will be explored.

Kevin Talbott George Mason University

Modeling the Evaporation of a Tear Film Over a Contact Lens

A contact lens (CL) is porous and thus fluid can flow between the post-lens tear film (PoLTF), which is the fluid between the corneal surface and the contact lens, and the pre-lens tear film (PrLTF), which is the fluid on top of the contact lens exposed to the air. We examine a model for a tear film in the presence of a contact lens which allows for fluid transfer through the lens and includes the effects of evaporation on the PrLTF. Evaporation depletes the PrLTF, and continued evaporation causes depletion of the PoLTF via fluid loss through the contact lens. Governing equations include Navier-Stokes equations, heat equation and Darcy's equation for the fluid flow and heat transfer in the fluid film and porous layer. A 1-D model reduces to an ODE that can be solved numerically or analytically. We explore these issues more generally in a 2-D tear film model described by a PDE that is first order in time and fourth order in space.

Olivia Walch College of William and Mary

Modeling Facilitation and Depression in Thalamocortical Relay Neurons

Thalamocortical relay (TC) neurons in the lateral geniculate nucleus receive both retinal and cortical input; however, the two pre-synaptic signals are filtered in significantly different ways. Using a three-compartment model of a TC cell, with distinct equations for the proximal and distal dendrites, we model the facilitation of signals from the cortex and depression of input from the retina. Additionally, we present several model-generated cross-correlograms that lend insight into the interplay of the driving and modulating afferents.

Jeff Soosiah College of William and Mary

Perfect Partitioning of Sets of Permutations

Given sets of permutations as block permutation matrices of fixed dimensions, we conjecture that the set of all such permutations can be perfectly partitioned, for any choice of dimensions and block size. We demonstrate that the conjecture holds for specific choices of the dimension with block size 2×2 .

Ian Johnson George Mason University

Numerical Continuation with the Diblock Copolymer Equation in One Dimension

Diblock copolymers are a class of materials formed by the reaction of two linear polymers. The different structures taken on by these polymers grant them special properties, which can prove useful in applications such as development of new adhesives and asphalt additives. The diblock copolymer equation governs the formation of these polymers. Using the software package **AUTO**, numerical continuation was used to investigate the diblock copolymer equation in one dimension. In combination with direct simulation, a phase diagram of long-term behavior was constructed.

Ben Holman College of William and Mary

Patterns in Extinction in Coupled Ricker Model

Ecologists use Ricker patch models to study meta population dynamics for populations undergoing growth and dispersal in a patchy environment. We discuss a modified model in which patch-wise extinction thresholds are used to model local extinction events. Numerical simulations for certain parameters exhibit a decoupling of the system into small regions with periodic dynamics prior to extinction. To further analyze this high dimensional system we focus on computational homology as a tool for measuring spatial patterns as extinction occurs.

Russell Mahoney George Mason University

Modeling of Interface-Dominated Materials Properties

Many materials used today are polycrystalline aggregates composed of large numbers of minuscule grains. These grains are separated by grain boundaries which determine the properties of the material such as elasticity or conductivity. A combination of macro- and mesoscopic tools such as the finite element microstructure analysis package **00F2** and in-house grain growth models are used to perform a comprehensive of the dynamical effects grain coarsening has on these materials properties. By analyzing how these materials respond to stress, electricity, or heat, we hope to discover more about the impact of grain boundary distributions.

Ruoyan Sun College of William and Mary

Global Stability of Endemic Equilibrium of Multigroup SIR Model with Nonlinear Incidence

We introduce a basic reproduction number for a multigroup epidemic model with nonlinear incidence. Then, we establish that global dynamics are completely determined by the basic reproduction number R_0 . It shows that, the basic reproduction number R_0 is a global threshold parameter in the sense that if it is less than or equal to one, the disease free equilibrium is globally stable and the disease dies out; whereas if it is larger than one, there is a unique endemic equilibrium which is globally stable and thus the disease persists in the population.

Ari Cukierman College of William and Mary

Vertex Identifying Codes

The study of vertex identifying codes is grounded in graph theory and has applications in the design of multiprocessor networks. Roughly speaking, a vertex identifying code is a way of labeling the vertices of a graph. We are particularly interested in infinite graphs, *e.g.*, the square, triangular and hexagonal grids.

Arjun Sanghvi George Mason University

A Stability Study of an Equilibrium Asset Price Model

A previously developed heterogeneous agent model is used to simulate the price of a financial asset and successfully captures statistical properties standard to actual financial data. These stylized facts include: volatility clustering and the fat-tailed distribution of price changes. Such properties are absent from models that implement the neoclassical assumptions of economics such as geometric Brownian motion (gBm) with drift.

The proposed model invokes price thresholds to simulate agent behavior over a long timescale. Agents often act, rationally or irrationally, based on the choices of others in the system – often resulting in herding behavior. By introducing such effects into the gBm model, we control and thereby determine the effect of such variables on the market dynamics. Using herding as a bifurcation parameter we numerically study the stability of the revised model and find that for low levels of herding, the model loses stability; and as the level of herding is increased, the model achieves the most important stylized facts.

William Brayer George Mason University

An Agent-Based Modelling Approach to Financial Markets

Standard financial models are inadequate because they make very strong assumptions about rationality and efficiency that imply a Gaussian distribution of price changes. Yet bubbles and crashes frequently occur: thus conventional models severely underestimate the risk of extreme events in financial markets. The standard models use geometric Brownian motion to simulate the evolution of an asset price. We replace this pricing formula with an agent-based model whose demand changes with the asset price.

We describe simple rules governing the behavior of the agents that can mimic both the effects of (irrational) human psychology as well as systemic market defects that result in rational-but-perverse behavior. We show that technical analysis can produce excess returns and that herding may account for this phenomenon.

Georgia Pfeiffer College of William and Mary

Basins of Attraction in Stage Structured Populations

The interaction between invasive and native species can be modeled through a Lefkovich model using stage structured populations. In this study, we analyze population dynamics of a stage structured population, computing a basin of attraction around the non-trivial equilibrium. This model can be naturally extended to include two or more species in which inter- and intra-specific competition is expressed through a density dependent fertility term. Time permitting, preliminary results for the two species model will be permitted.

Dian Yang College of William and Mary

A Solvable Hyperbolic Free Boundary Problem Modeling Tumor Regrowth

Recently Tian and Friedman et al. developed a mathematical model on brain tumor recurrence after resection. The model is a free boundary problem with a hyperbolic system of nonlinear partial differential equations. In this paper, we conduct a rigorous analysis on this hyperbolic system and prove the local and global existence and uniqueness of the solution. It is well known that most nonlinear free boundary problems are impossible to solve in terms of explicit analytical solutions. In contrast, the free boundary problem in this study is solvable, and the explicit solution is found by using the backward characteristic curve method. This explicit solution is then validated by numerical simulation results. An interesting finding in this study is that the problem can be treated as a hyperbolic system defined on an infinite domain where the initial condition has a first-type discontinuity. This is a joint work with Paul Tian (W& M) and Jin Wang (ODU).

Robert Hill George Mason University

Modeling Complex Physical Phenomena using Energy Minimization Principle

Modern modeling languages and optimization tools make it possible to analyze complex physical phenomena. The following two examples are driven by the energy minimization principle. First, we consider a problem of docking a molecular wire to a bacterial photosynthetic reaction center. To assemble efficient photovoltaic devices, it is critically important to explore how to dock highly conducting molecular wires to the RC. Second, we consider the problem of constructing phase diagrams, which is very important in materials science.

Byong Kwon George Mason University

Computational Docking of Molecular Wires to the Reaction Center of Rhodobacter Sphaeroides

Given the worldwide interest in renewable energy, scientists have been exploring the possibility of using bacterial photosynthetic reaction centers to build a new generation of highly efficient photovoltaic devices. To build such devices, molecular wires (MWs) that serve as good conductors to transport electrons from and to the reaction centers are needed. The MWs must dock at specific binding sites within the reaction centers.

We explore computational models of docking MWs to the reaction centers. Such models can help in proposing suitable MWs for photovoltaic devices. For our modeling, we use the reaction center of Rhodobacter sphaeroides, a purple photosynthetic bacteria.

Matt Peppe College of William and Mary

Assortativity in Networks of Neurons

A group of connected neurons can be represented as a directed graph with each neuron represented as a node and every connection from the axon of one neuron to the dendrite of another as a directed edge from the former to the latter. Directed graphs may display various forms of assortativity such as node-degree correlation. This talk covers ODE models of such networks and results obtained by numerically simulating them.